wwPDB EM Validation Summary Report (i)

Feb 11, 2024 – 09:35 PM EST

PDB ID	:	3EDL
EMDB ID	:	EMD-5027
Title	:	Kinesin13-Microtubule Ring complex
Authors	:	Tan, D.; Rice, W.J.; Sosa, H.
Deposited on	:	2008-09-03
Resolution	:	28.00 Å(reported)

This is a wwPDB EM Validation Summary Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (1)) were used in the production of this report:

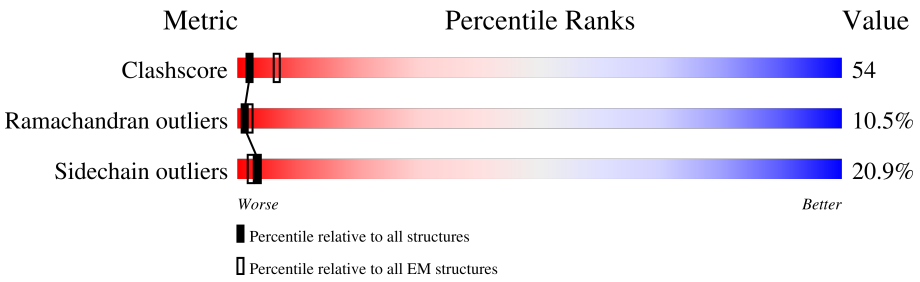
EMDB validation analysis	:	0.0.1.dev70
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 28.00 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion < 40%). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	451	22%; 16%, 57%, 17%, • , 9%
2	B	445	19%; 20%, 55%, 18%, • , •
2	G	445	12%; 37%, 35%, 19%, • , 6%
3	D	331	7%; 55%, 32%, • , 9%
4	F	451	8%; 38%, 37%, 16%, • , 7%

2 Entry composition (i)

There are 12 unique types of molecules in this entry. The entry contains 15757 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Tubulin alpha-1A chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	412	3227	2043	551	613	20	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	265	GLY	ALA	conflict	UNP P02550

- Molecule 2 is a protein called Beta tubulin.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	426	3351	2105	575	646	25	0	0
2	G	419	3237	2037	544	631	25	0	0

- Molecule 3 is a protein called Kinesin-like protein KIF2C.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	D	301	2368	1496	416	438	18	0	0

- Molecule 4 is a protein called Tubulin alpha-1A chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	F	421	3220	2043	544	612	21	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	265	ILE	ALA	conflict	UNP P02550

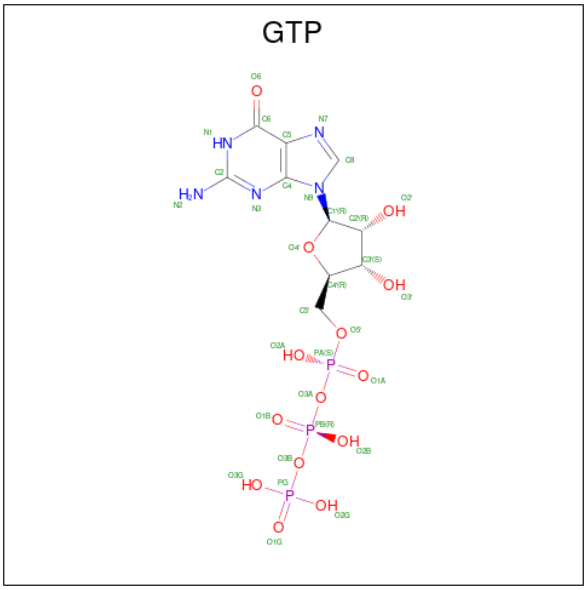
- Molecule 5 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
			Total	Zn	
5	A	1	1	1	0

- Molecule 6 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

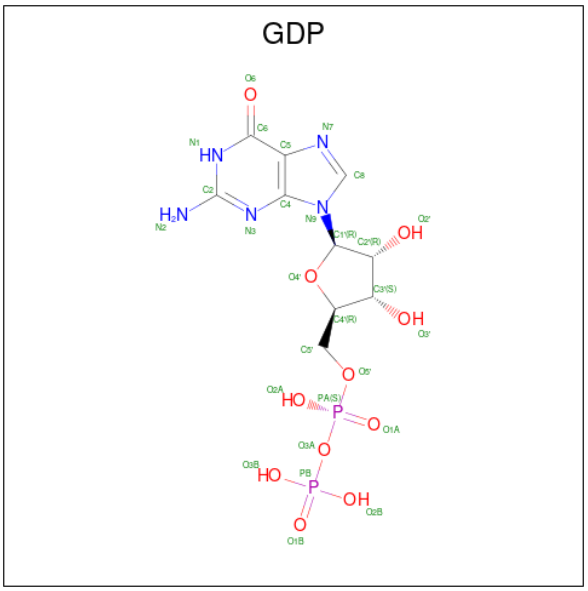
Mol	Chain	Residues	Atoms		AltConf
			Total	Mg	
6	A	1	1	1	0
6	D	1	Total	Mg	0
			1	1	
6	F	1	Total	Mg	0
			1	1	

- Molecule 7 is GUANOSINE-5'-TRIPHOSPHATE (three-letter code: GTP) (formula: $C_{10}H_{16}N_5O_{14}P_3$).



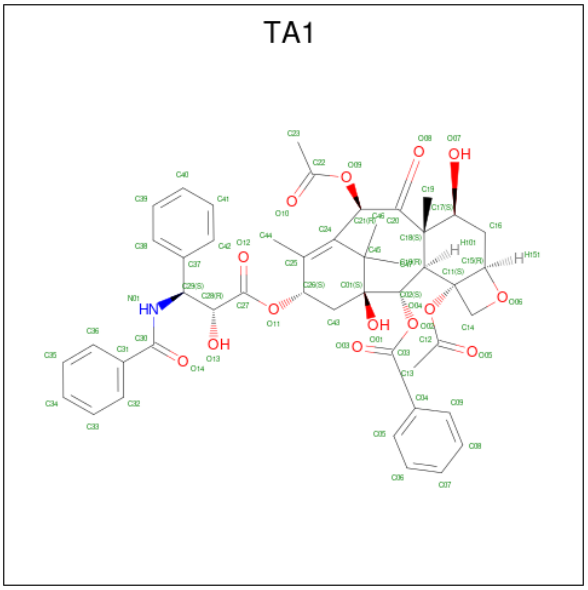
Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
7	B	1	32	10	5	14	3	0
7	F	1	Total	C	N	O	P	0
			32	10	5	14	3	

- Molecule 8 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula: $C_{10}H_{15}N_5O_{11}P_2$).



Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
8	B	1	28	10	5	11	2	0
			Total	C	N	O	P	
8	F	1	28	10	5	11	2	0

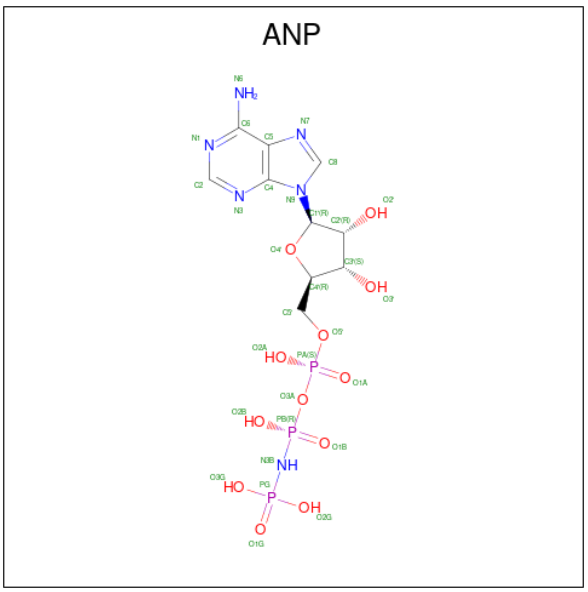
- Molecule 9 is TAXOL (three-letter code: TA1) (formula: $C_{47}H_{51}NO_{14}$).



Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
9	B	1	62	47	1	14	0

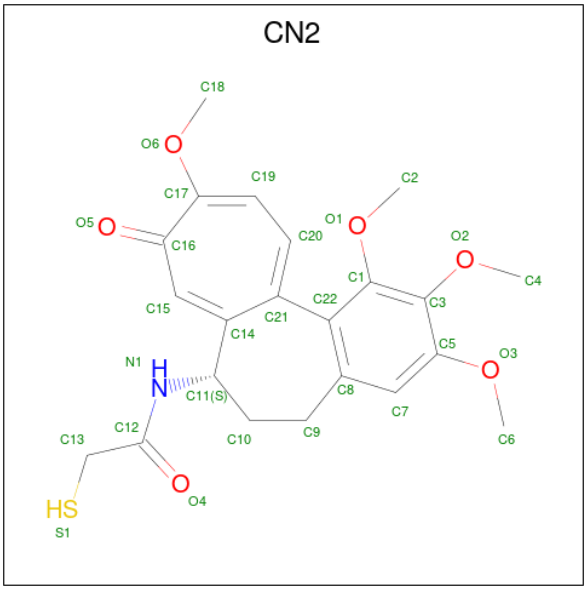
- Molecule 10 is PHOSPHOAMINOPHOSPHONIC ACID-ADENYLATE ESTER (three-

letter code: ANP) (formula: $C_{10}H_{17}N_6O_{12}P_3$).



Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
10	D	1	31	10	6	12	3	0

- Molecule 11 is 2-MERCAPTO-N-[1,2,3,10-TETRAMETHOXY-9-OXO-5,6,7,9-TETRA HYDRO-BENZO[A]HEPTALEN-7-YL]ACETAMIDE (three-letter code: CN2) (formula: $C_{22}H_{25}NO_6S$).



Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	S	
11	G	1	30	22	1	6	1	0

- Molecule 12 is water.

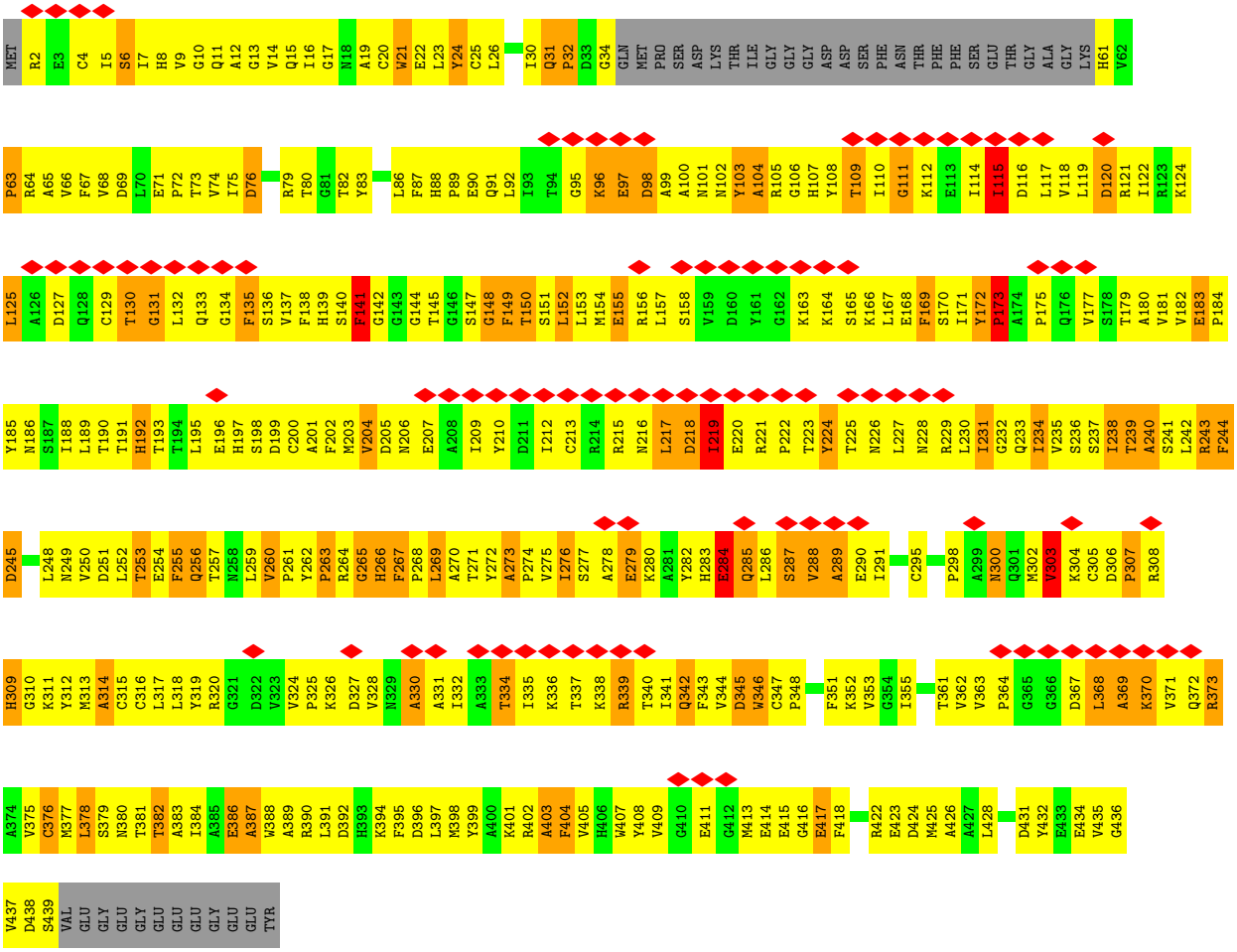
Mol	Chain	Residues	Atoms		AltConf
			Total	O	
12	D	98	98	98	0
			Total	O	
12	F	9	9	9	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

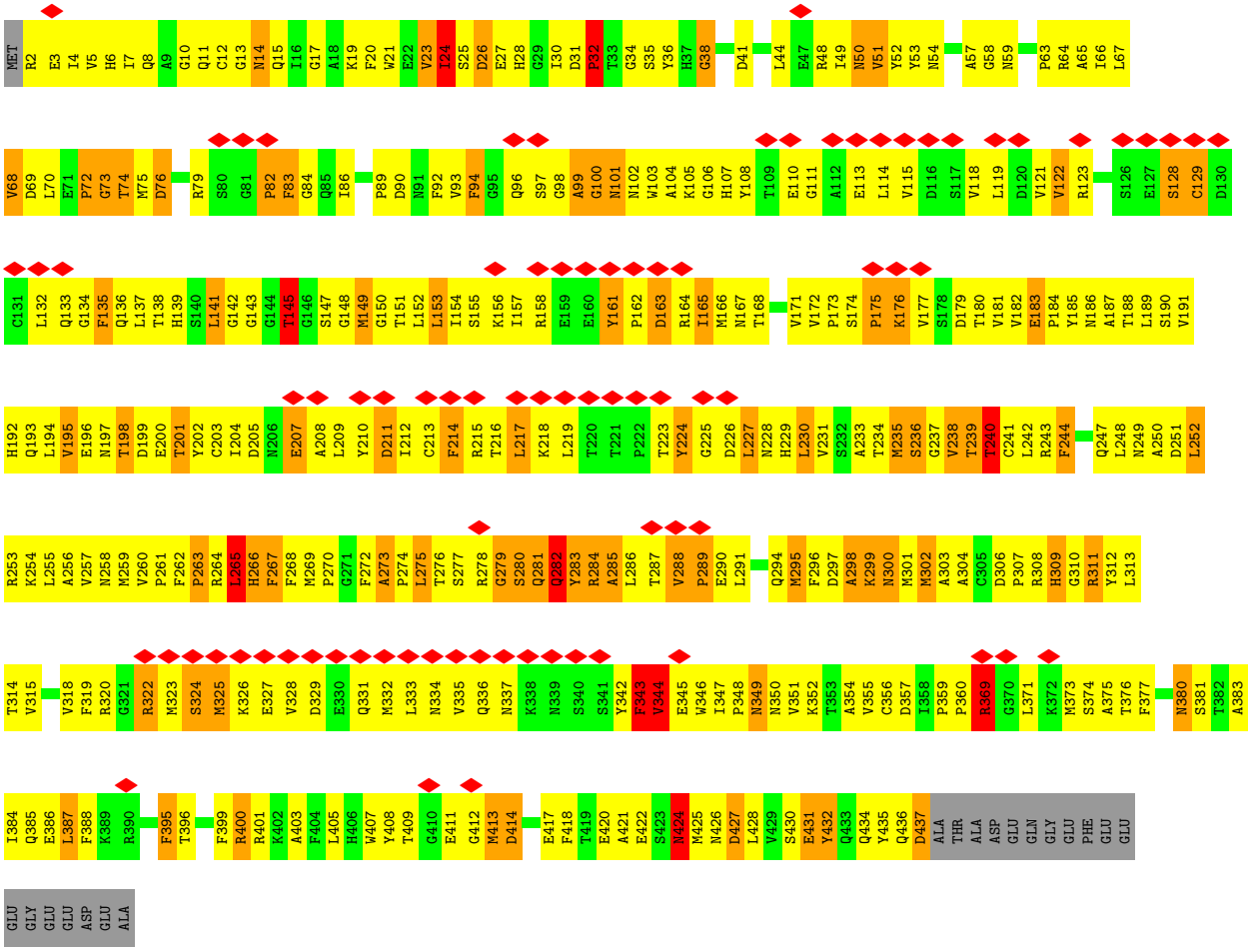
- Molecule 1: Tubulin alpha-1A chain

Chain A: 22% 16% 57% 17% • 9%



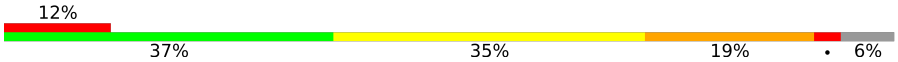
- Molecule 2: Beta tubulin

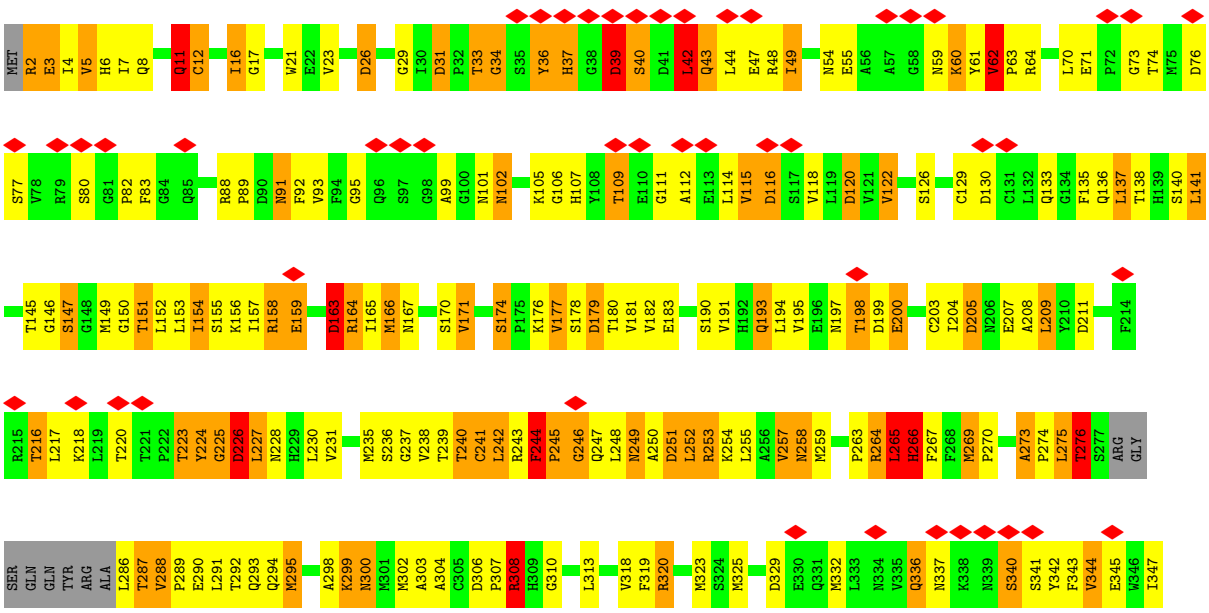
Chain B: 19% 20% 55% 18% • •

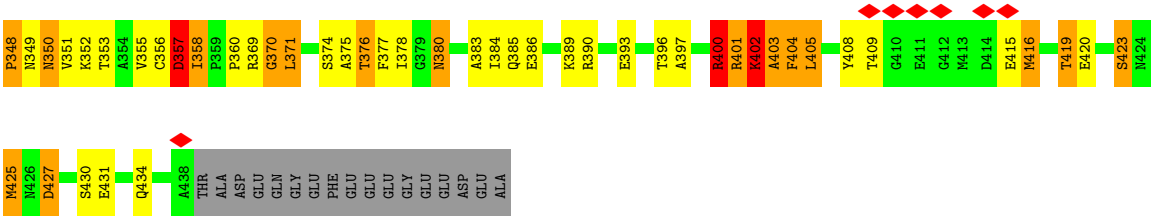


- Molecule 2: Beta tubulin

Chain G:

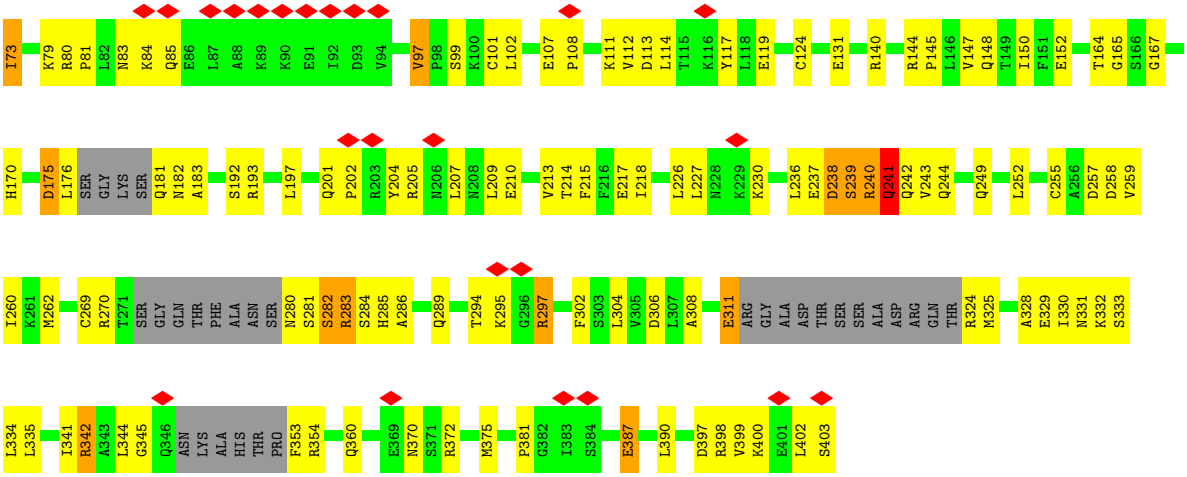






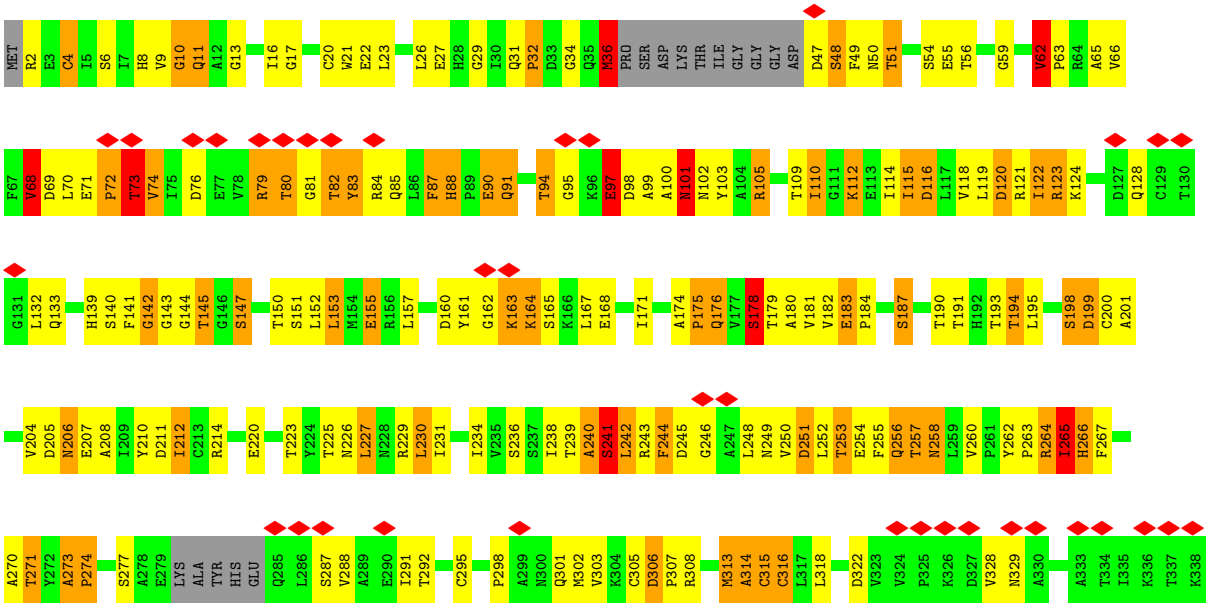
- Molecule 3: Kinesin-like protein KIF2C

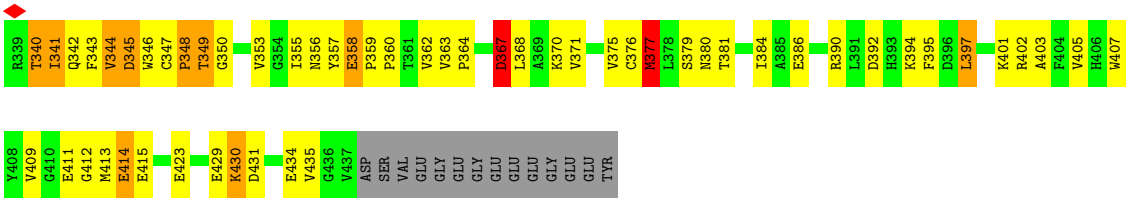
Chain D:



- Molecule 4: Tubulin alpha-1A chain

Chain F:




R339
T340
I341
Q342
F343
V344
D345
W346
C347
P348
T349
G350
V353
G354
I355
N356
Y357
E358
P359
P360
T361
V362
V363
P364
D367
L368
A369
K370
V371
V375
C376
W377
L378
S379
N380
T381
I384
A385
E386
R390
L391
D392
H393
K394
F395
D396
L397
K401
R402
A403
F404
V405
H406
W407
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V409
G410
E411
G412
M413
E414
E415
E423
E429
K430
D431
E434
V435
G436
V437
ASP
SER
VAL
GLU
GLY
GLU
GLY
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GLU
GLU
GLY
GLU
GLU
TYR

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	HELICAL	Depositor
Imposed symmetry	HELICAL, twist=Not provided°, rise=Not provided Å, axial sym=Not provided	Depositor
Number of segments used	Not provided	
Resolution determination method	Not provided	
CTF correction method	Each particle	Depositor
Microscope	FEI TECNAI F20	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/Å^2$)	Not provided	
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	50000	Depositor
Image detector	KODAK SO-163 FILM	Depositor
Maximum map value	55.000	Depositor
Minimum map value	-48.000	Depositor
Average map value	0.563	Depositor
Map value standard deviation	12.837	Depositor
Recommended contour level	11.1	Depositor
Map size (Å)	606.0, 606.0, 246.0	wwPDB
Map dimensions	101, 101, 41	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	6.0, 6.0, 6.0	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, MG, GTP, CN2, GDP, TA1, ANP

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\|>5$	RMSZ	$\#\|Z\|>5$
1	A	0.51	0/3300	0.73	0/4482
2	B	0.51	0/3426	0.76	2/4642 (0.0%)
2	G	0.61	0/3309	1.00	20/4494 (0.4%)
3	D	0.46	0/2398	0.71	2/3217 (0.1%)
4	F	0.66	2/3292 (0.1%)	0.95	15/4479 (0.3%)
All	All	0.56	2/15725 (0.0%)	0.84	39/21314 (0.2%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	F	97	GLU	CD-OE1	-6.53	1.18	1.25
4	F	97	GLU	CD-OE2	-5.40	1.19	1.25

The worst 5 of 39 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	F	160	ASP	CB-CG-OD2	6.88	124.49	118.30
2	G	205	ASP	CB-CG-OD2	6.84	124.45	118.30
2	G	163	ASP	CB-CG-OD2	6.73	124.36	118.30
4	F	244	PHE	N-CA-C	6.73	129.17	111.00
2	G	116	ASP	CB-CG-OD2	6.32	123.99	118.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen

atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3227	0	3143	548	0
2	B	3351	0	3229	545	0
2	G	3237	0	3060	269	0
3	D	2368	0	2410	219	0
4	F	3220	0	3074	232	0
5	A	1	0	0	0	0
6	A	1	0	0	0	0
6	D	1	0	0	0	0
6	F	1	0	0	0	0
7	B	32	0	12	4	0
7	F	32	0	12	2	0
8	B	28	0	12	1	0
8	F	28	0	12	1	0
9	B	62	0	51	6	0
10	D	31	0	13	3	0
11	G	30	0	23	8	0
12	D	98	0	0	4	0
12	F	9	0	0	10	0
All	All	15757	0	15051	1665	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 54.

The worst 5 of 1665 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:238:ASP:CA	2:G:419:THR:HB	1.24	1.61
3:D:236:LEU:CD2	2:G:416:MET:CE	2.11	1.28
3:D:237:GLU:O	2:G:420:GLU:HA	1.30	1.28
3:D:238:ASP:CB	2:G:419:THR:HB	1.63	1.27
3:D:112:VAL:HG11	4:F:435:VAL:CG2	1.62	1.27

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	408/451 (90%)	266 (65%)	83 (20%)	59 (14%)	0 4
2	B	424/445 (95%)	273 (64%)	95 (22%)	56 (13%)	0 5
2	G	415/445 (93%)	310 (75%)	57 (14%)	48 (12%)	0 6
3	D	291/331 (88%)	275 (94%)	13 (4%)	3 (1%)	15 55
4	F	415/451 (92%)	316 (76%)	59 (14%)	40 (10%)	0 10
All	All	1953/2123 (92%)	1440 (74%)	307 (16%)	206 (10%)	1 8

5 of 206 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	96	LYS
1	A	97	GLU
1	A	108	TYR
1	A	109	THR
1	A	141	PHE

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	347/377 (92%)	298 (86%)	49 (14%)	3 16
2	B	367/381 (96%)	307 (84%)	60 (16%)	2 13
2	G	348/381 (91%)	241 (69%)	107 (31%)	0 2
3	D	261/286 (91%)	237 (91%)	24 (9%)	9 29

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
4	F	336/378 (89%)	229 (68%)	107 (32%)	0 2
All	All	1659/1803 (92%)	1312 (79%)	347 (21%)	3 6

5 of 347 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	F	384	ILE
2	G	177	VAL
4	F	415	GLU
2	G	76	ASP
2	G	230	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 60 such sidechains are listed below:

Mol	Chain	Res	Type
3	D	182	ASN
2	G	300	ASN
4	F	88	HIS
2	G	294	GLN
2	G	385	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains (i)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 11 ligands modelled in this entry, 4 are monoatomic - leaving 7 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and

the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
8	GDP	F	603	-	24,30,30	1.24	2 (8%)	30,47,47	1.57	7 (23%)
7	GTP	B	500	6	26,34,34	1.31	4 (15%)	32,54,54	1.11	3 (9%)
7	GTP	F	601	6	26,34,34	1.22	2 (7%)	32,54,54	1.70	9 (28%)
9	TA1	B	601	-	68,68,68	2.01	19 (27%)	105,105,105	1.39	11 (10%)
10	ANP	D	500	6	29,33,33	1.69	4 (13%)	31,52,52	3.40	12 (38%)
11	CN2	G	701	-	27,32,32	3.27	7 (25%)	26,45,45	5.00	11 (42%)
8	GDP	B	600	-	24,30,30	2.59	9 (37%)	30,47,47	2.92	8 (26%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	GDP	F	603	-	-	3/12/32/32	0/3/3/3
7	GTP	B	500	6	-	3/18/38/38	0/3/3/3
7	GTP	F	601	6	-	4/18/38/38	0/3/3/3
9	TA1	B	601	-	-	9/41/127/127	0/7/7/7
10	ANP	D	500	6	-	9/14/38/38	0/3/3/3
11	CN2	G	701	-	-	2/10/27/27	0/3/3/3
8	GDP	B	600	-	-	4/12/32/32	0/3/3/3

The worst 5 of 47 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	G	701	CN2	C20-C19	-8.49	1.24	1.38
11	G	701	CN2	C19-C17	-7.83	1.25	1.39
11	G	701	CN2	C15-C16	7.34	1.54	1.39
11	G	701	CN2	C20-C21	-6.77	1.24	1.39
8	B	600	GDP	O4'-C1'	6.20	1.49	1.41

The worst 5 of 61 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	G	701	CN2	C19-C20-C21	20.64	146.64	129.68
8	B	600	GDP	C8-N7-C5	9.27	120.65	102.99
11	G	701	CN2	C10-C11-N1	-8.94	93.97	110.04
10	D	500	ANP	O2B-PB-O1B	8.58	127.91	109.92
10	D	500	ANP	O5'-PA-O1A	-7.67	79.12	109.07

There are no chirality outliers.

5 of 34 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	F	601	GTP	C5'-O5'-PA-O1A
8	B	600	GDP	PA-O3A-PB-O2B
8	B	600	GDP	C5'-O5'-PA-O3A
8	B	600	GDP	C5'-O5'-PA-O1A
10	D	500	ANP	PG-N3B-PB-O1B

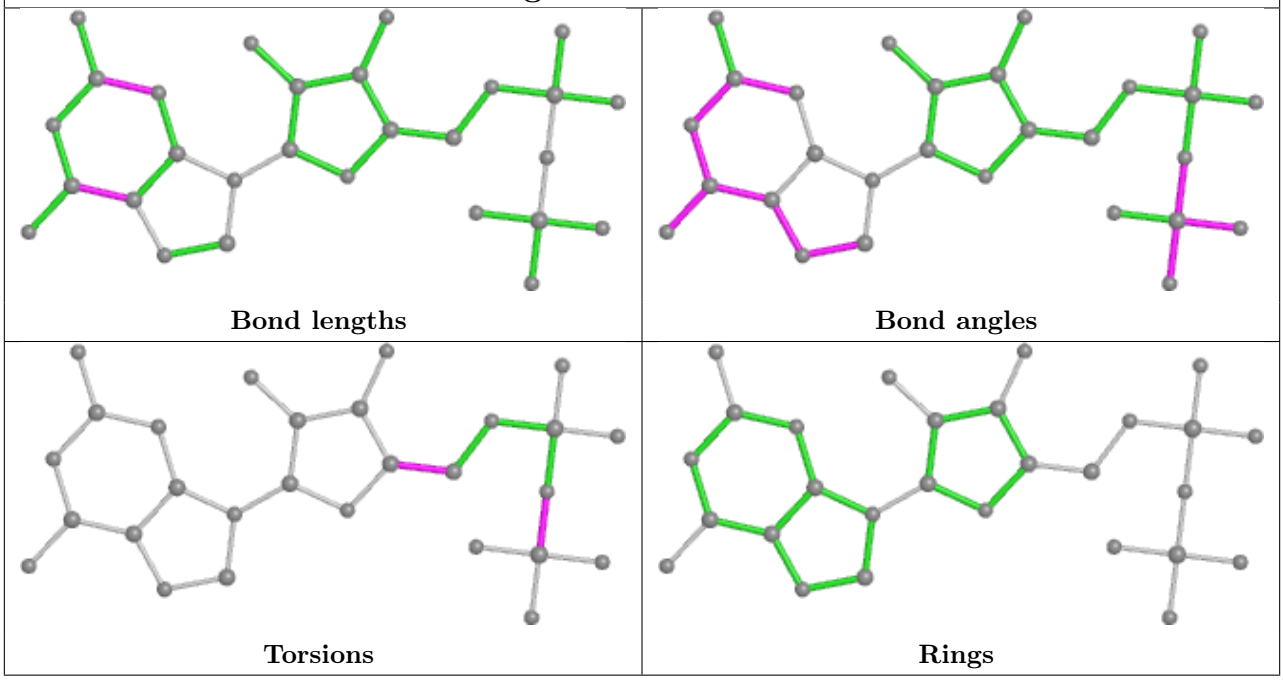
There are no ring outliers.

7 monomers are involved in 25 short contacts:

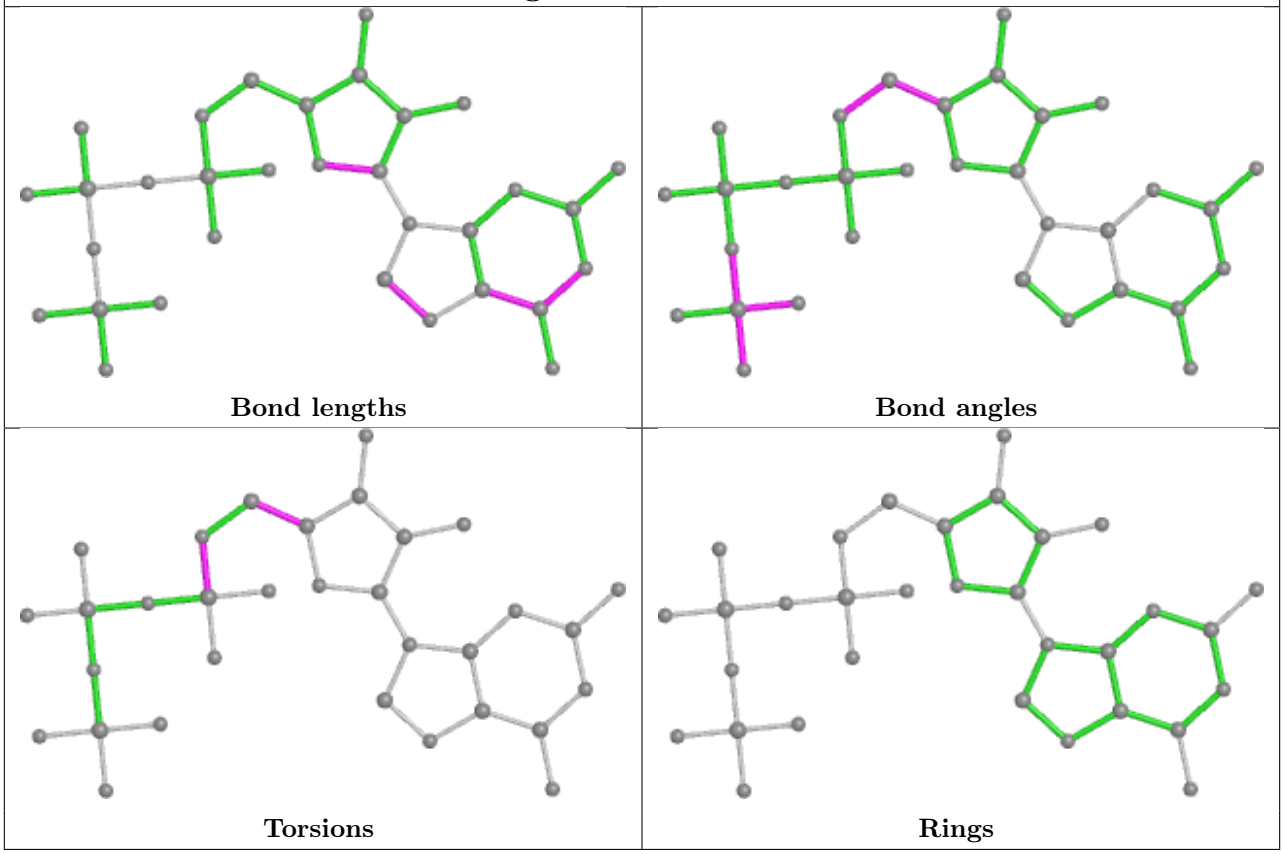
Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	F	603	GDP	1	0
7	B	500	GTP	4	0
7	F	601	GTP	2	0
9	B	601	TA1	6	0
10	D	500	ANP	3	0
11	G	701	CN2	8	0
8	B	600	GDP	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

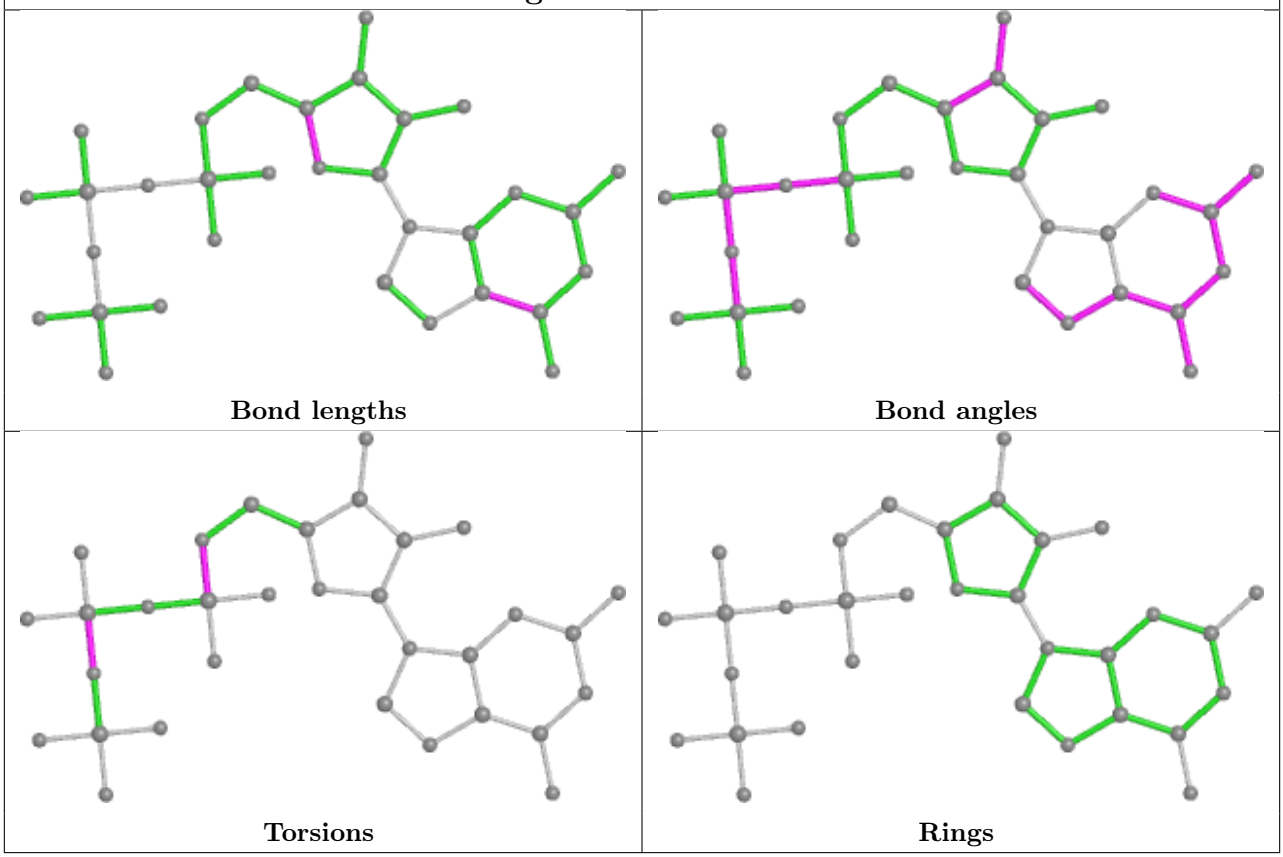
Ligand GDP F 603



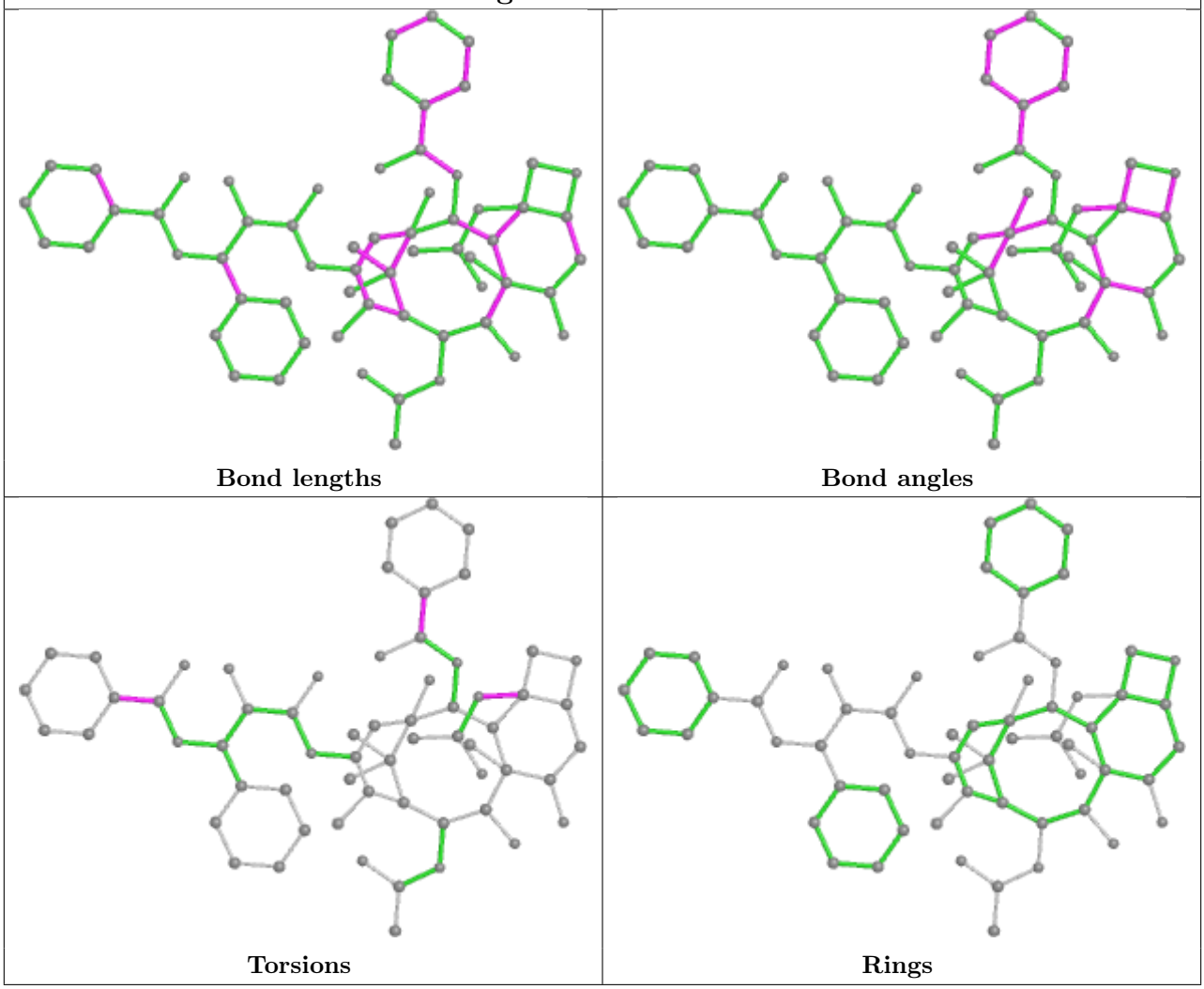
Ligand GTP B 500



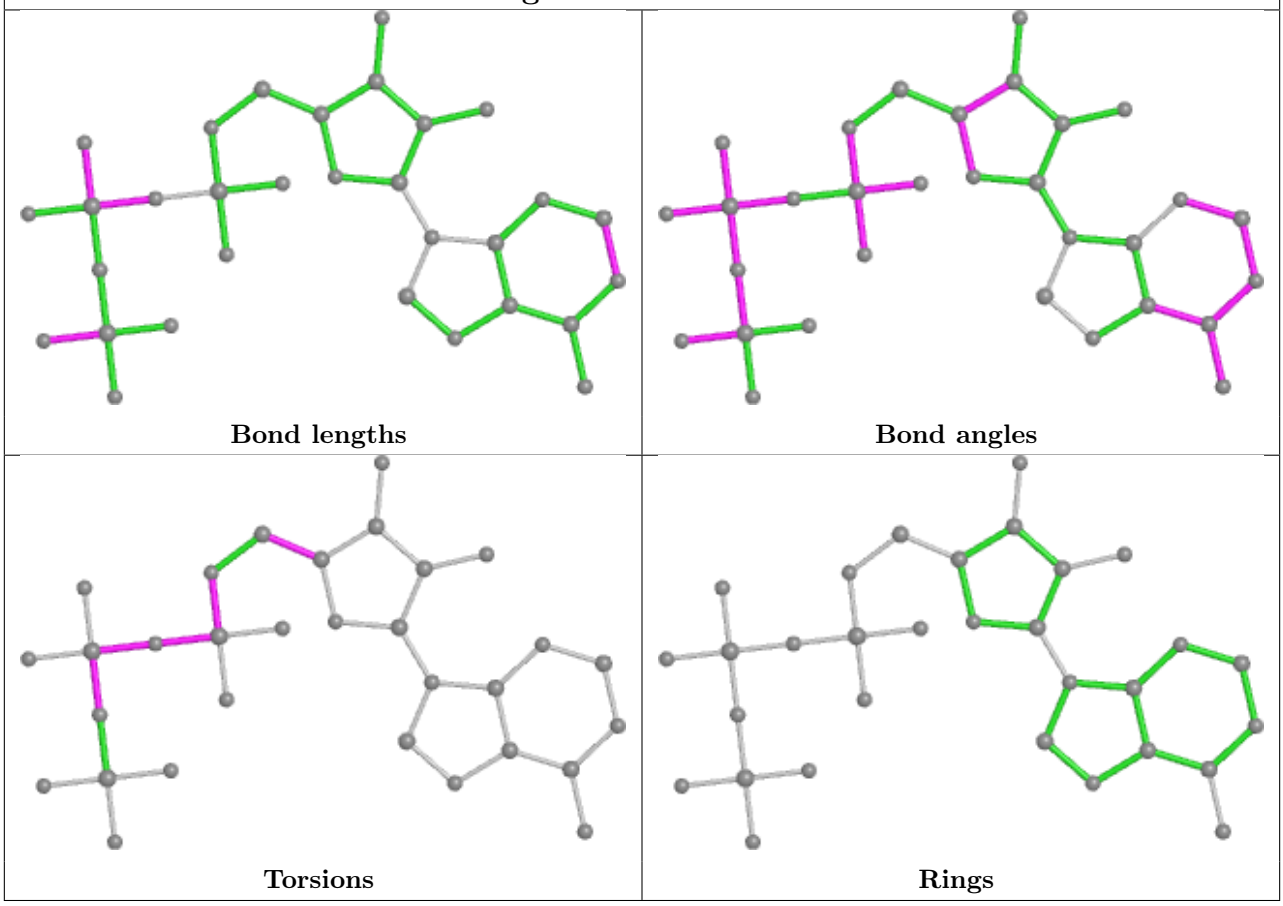
Ligand GTP F 601



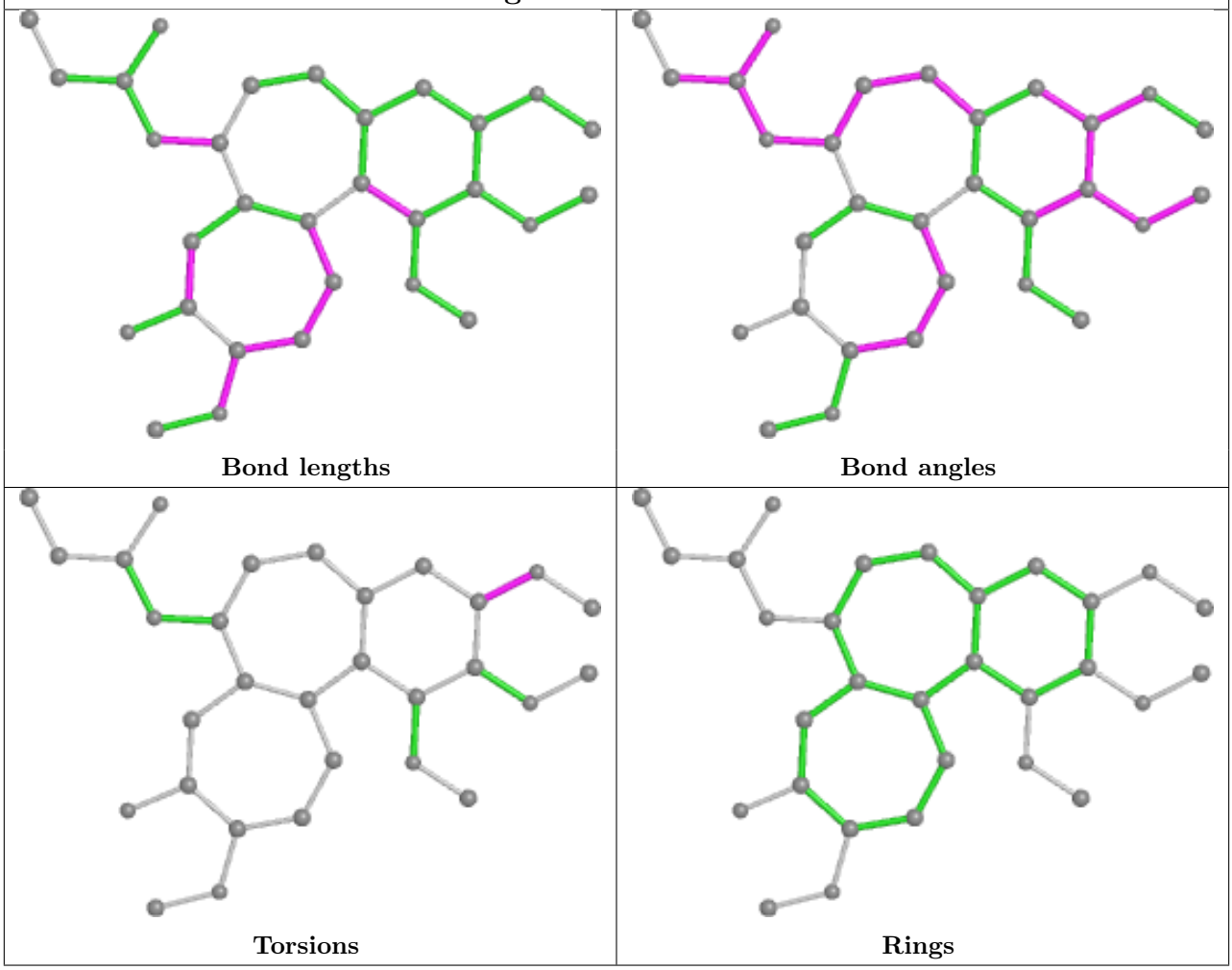
Ligand TA1 B 601



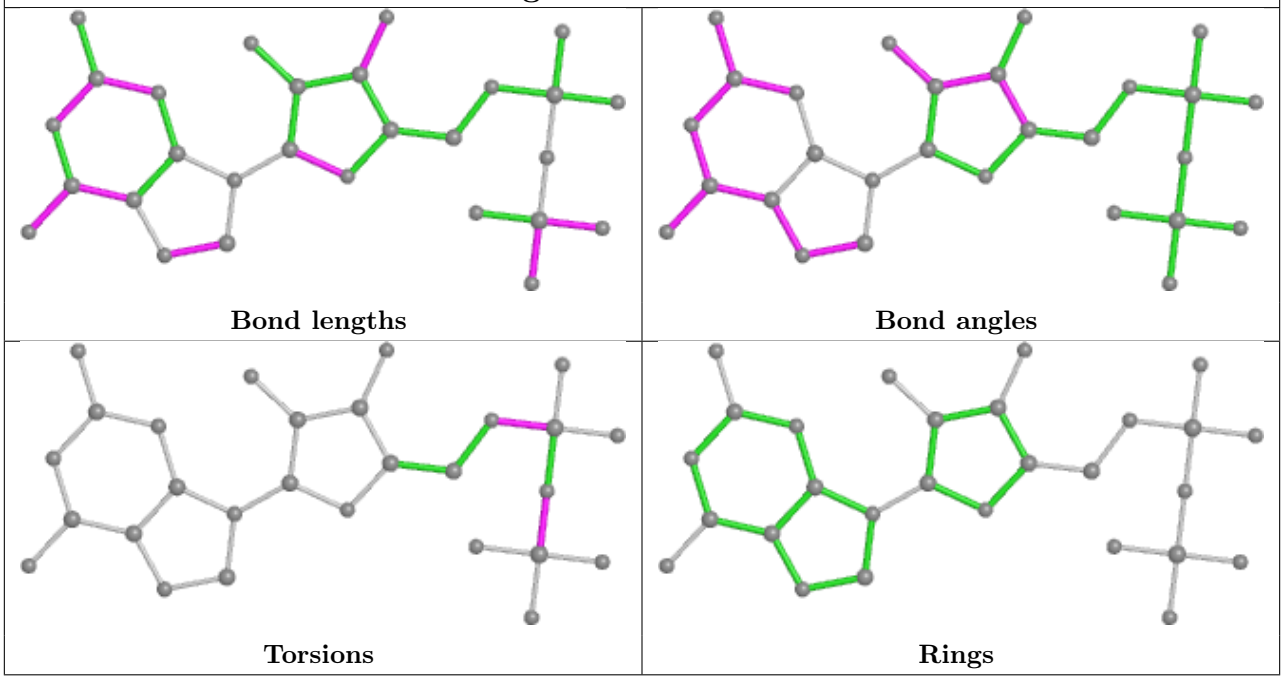
Ligand ANP D 500



Ligand CN2 G 701



Ligand GDP B 600



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

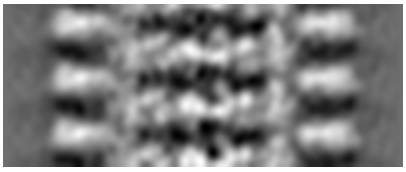
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-5027. These allow visual inspection of the internal detail of the map and identification of artifacts.

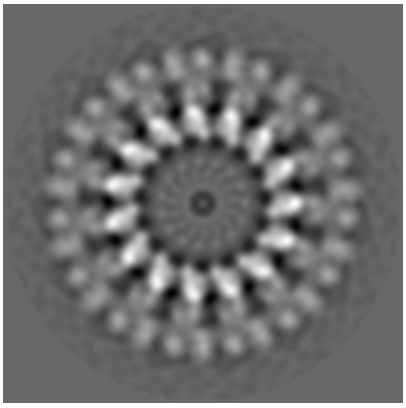
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections (i)

6.1.1 Primary map


X

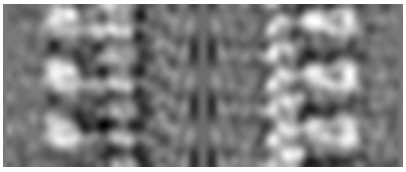
Y


Z

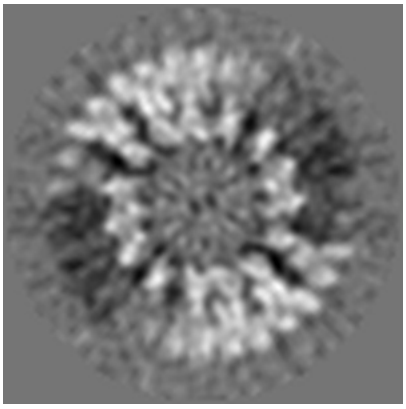
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

6.2.1 Primary map


X Index: 50

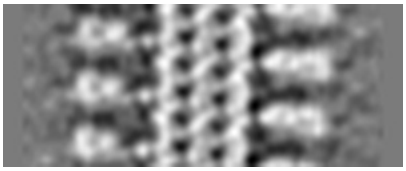
Y Index: 50


Z Index: 20

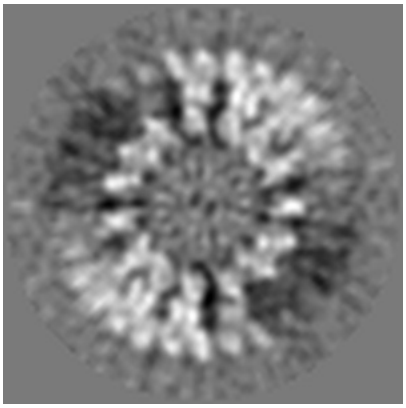
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

6.3.1 Primary map


X Index: 71

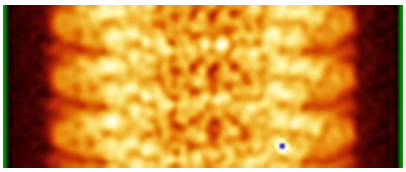
Y Index: 69

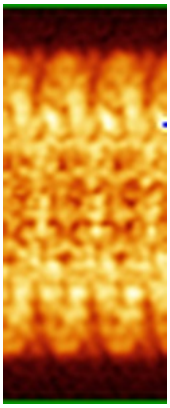

Z Index: 24

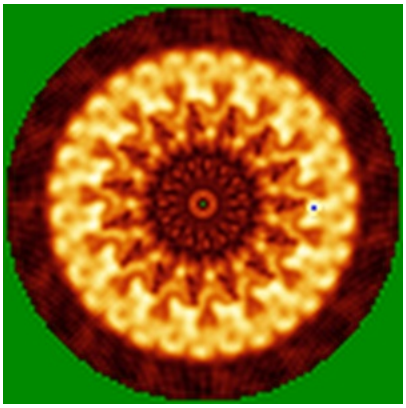
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) (i)

6.4.1 Primary map


X

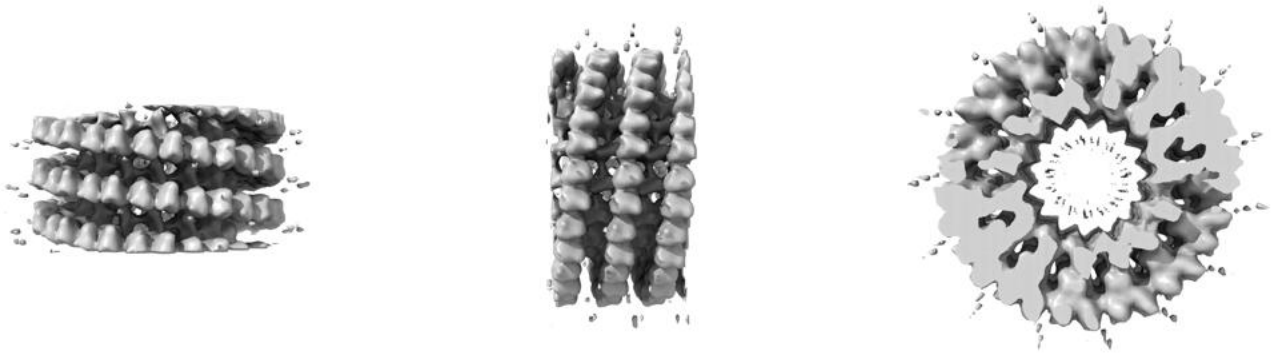

Y


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views (i)

6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 11.1. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

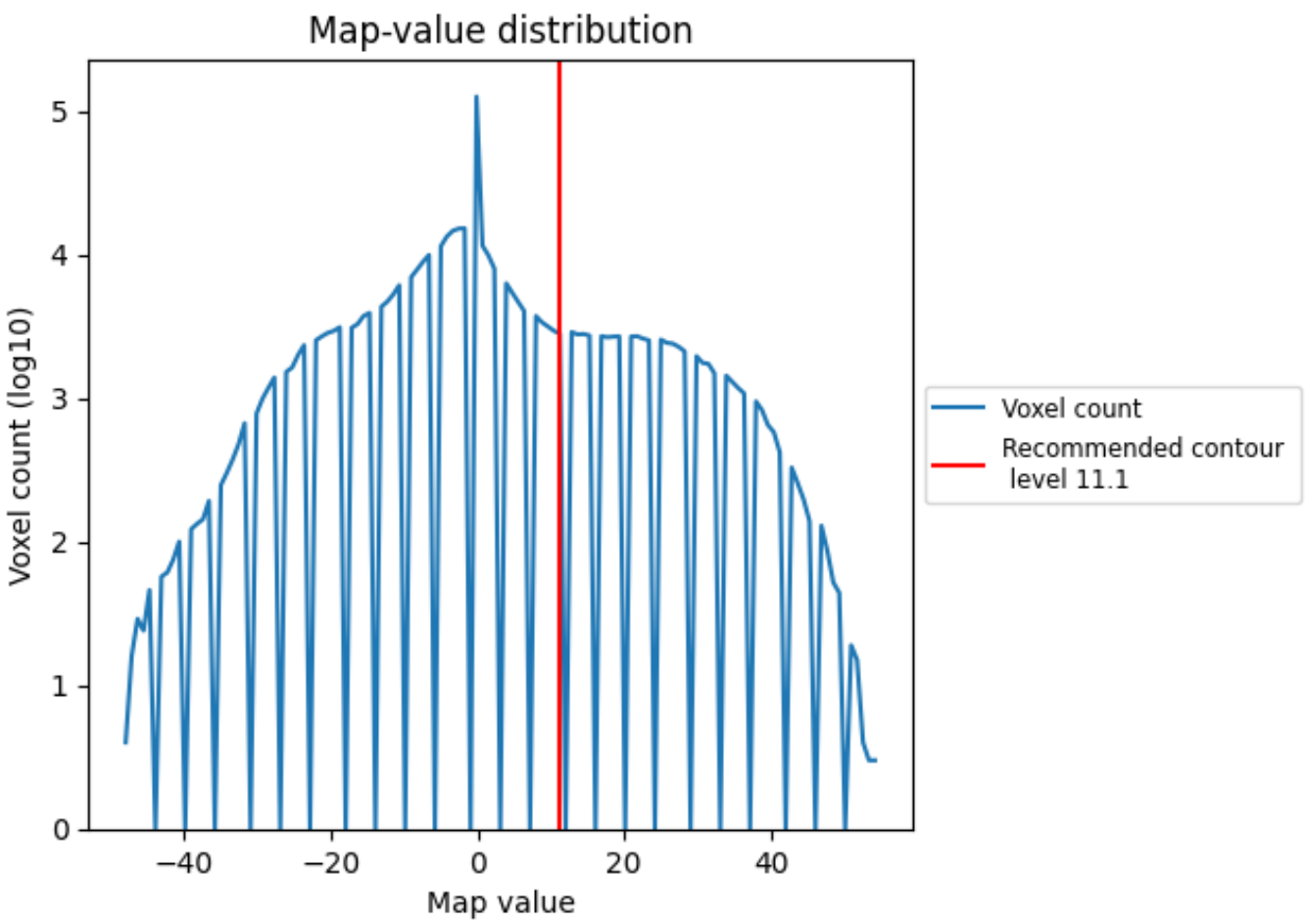
6.6 Mask visualisation (i)

This section was not generated. No masks/segmentation were deposited.

7 Map analysis (i)

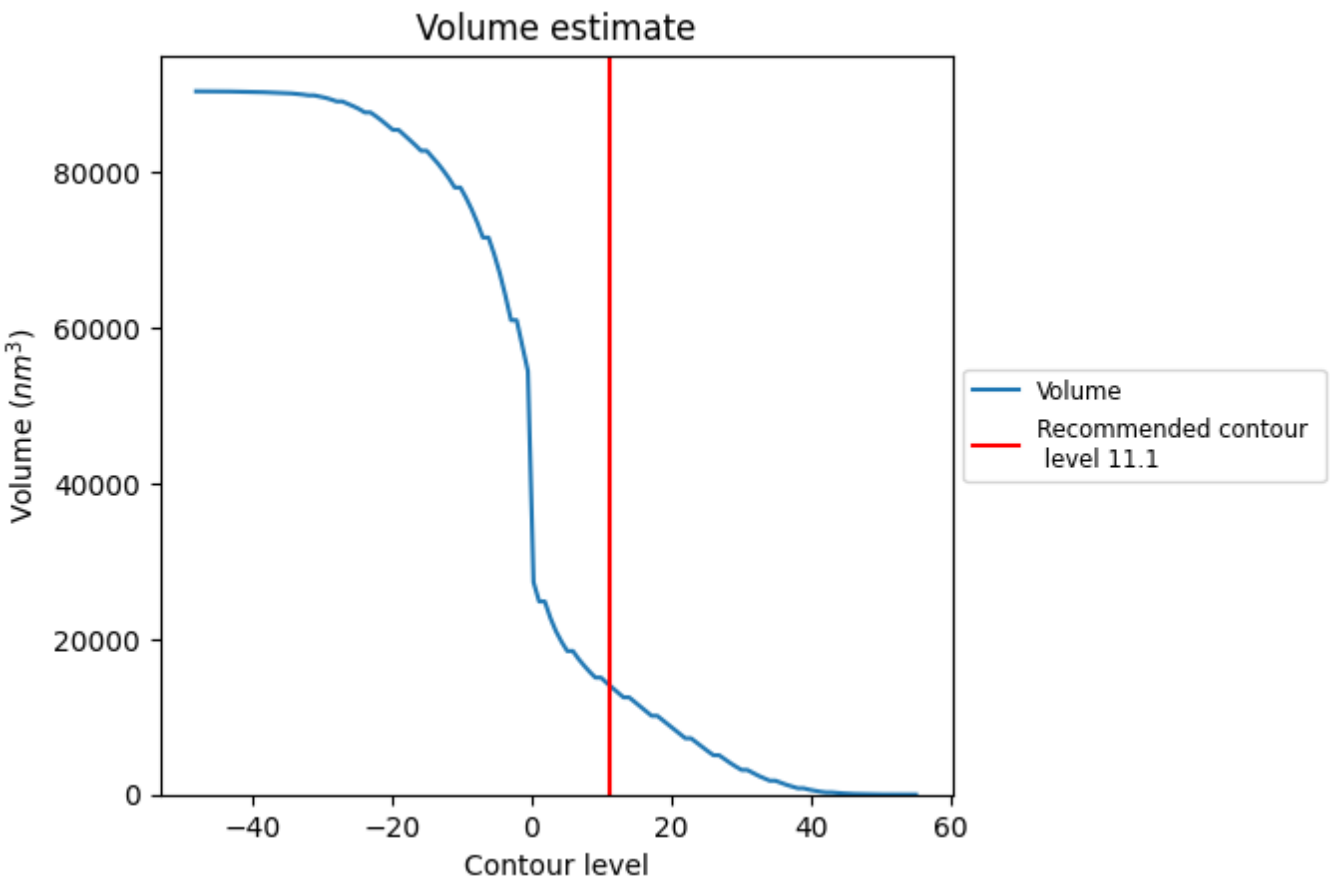
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution (i)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

7.2 Volume estimate (i)



The volume at the recommended contour level is 14065 nm^3; this corresponds to an approximate mass of 12705 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum (i)

This section was not generated. The rotationally averaged power spectrum is only generated for cubic maps.

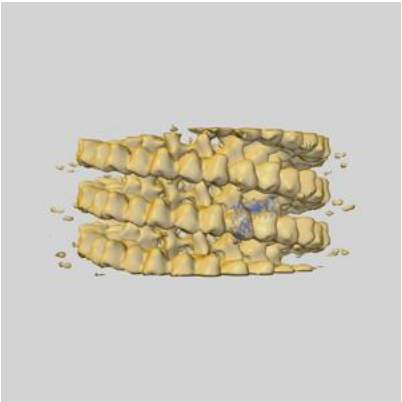
8 Fourier-Shell correlation (i)

This section was not generated. No FSC curve or half-maps provided.

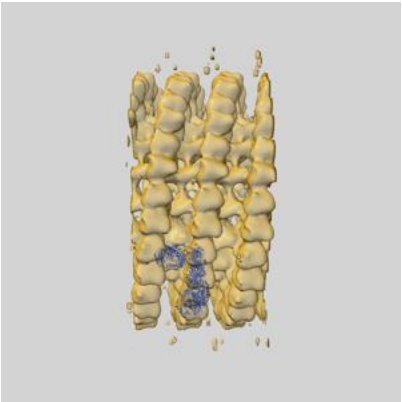
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-5027 and PDB model 3EDL. Per-residue inclusion information can be found in section 3 on page 8.

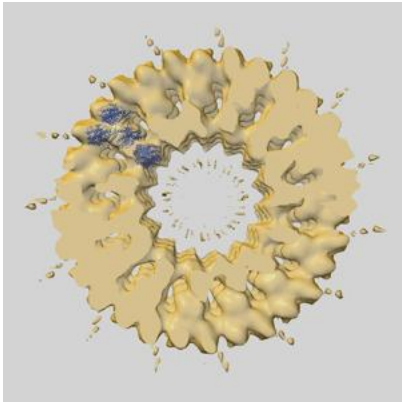
9.1 Map-model overlay (i)



X



Y



Z

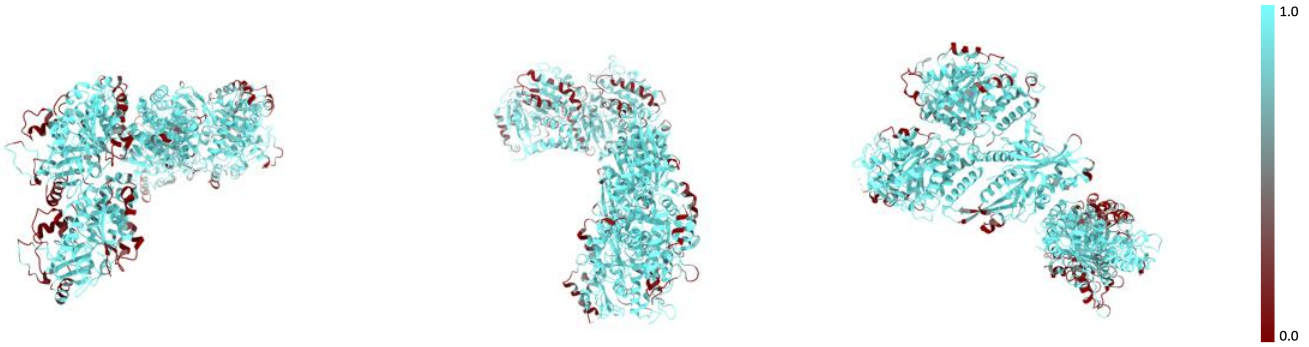
The images above show the 3D surface view of the map at the recommended contour level 11.1 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model (i)

X Y Z

The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

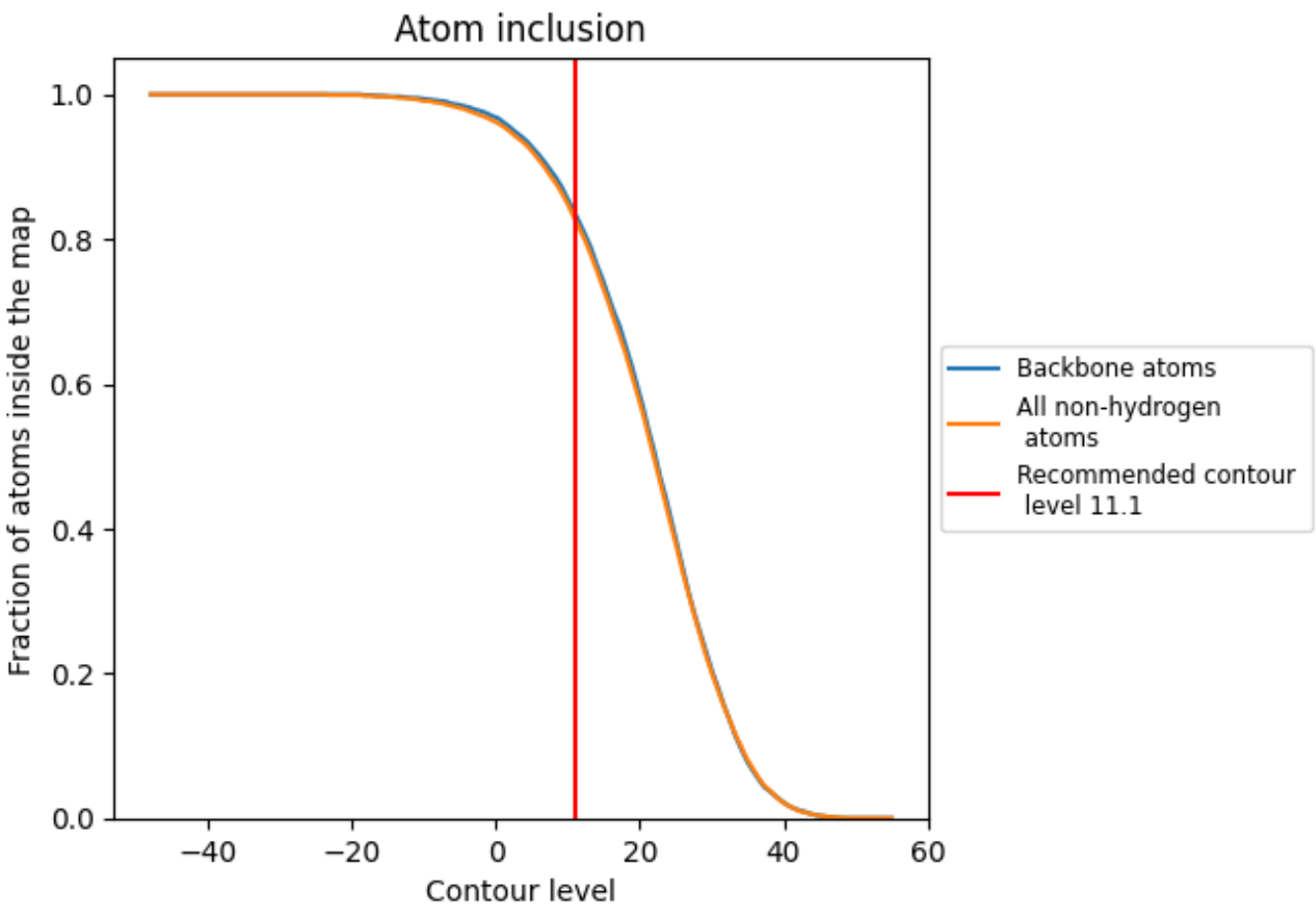
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (11.1).

9.4 Atom inclusion (i)



At the recommended contour level, 83% of all backbone atoms, 82% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (11.1) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8250	0.0440
A	0.7400	0.0440
B	0.7690	0.0400
D	0.8900	0.0490
F	0.9020	0.0460
G	0.8470	0.0430